

Applicability of an Iterative Inversion Algorithm to the Diffraction Patterns from Inhomogeneously Strained Crystals

A. A. Minkevich,^{*} M. Gailhanou, O. Thomas

TECSEN, UMR CNRS 6122, Université Paul Cézanne, 13397 Marseille, France

A lot of progress has been made lately on the development of iterative inversion algorithms for retrieving the shape of crystals directly from their diffraction pattern [1, 2]. In the case of strained crystals the convergence of the algorithms is more difficult. It is, however, a very important issue to evaluate local strains in nano-materials since these strains can have a great influence on various physical properties. We present here new numerical procedures, which allow for direct inversion of displacement fields in highly inhomogeneously strained objects.

In the case of a strained object, the direct space density can be expressed as a complex-valued number, whose phase provides information, within some small approximations, about the projection $u_{||}$ of the displacement field along the direction of momentum transfer vector \vec{q} . The iterative algorithm mentioned above for inverting reciprocal space maps from such types of objects has been investigated. It is observed that in the case of complex valued numbers expressing the highly inhomogeneously strained crystal density the convergence of the algorithms is problematic since ambiguity in solutions appears yielding to enormous numbers of local minima with very small error metric [3]. It means that different combinations of amplitudes and phases in direct space yield very similar Fourier transform amplitudes images. Therefore without additional *a priori* knowledge the "phase problem" proves to be difficult to solve by this approach in the case of inhomogeneously strained crystals.

Here a new method is proposed to break this stagnation. It is based on the use of additional but reasonable constraints in direct space, such as the maximal value of the displacement field derivatives [3]. This information can be approximately estimated from the diffracted intensity map. The method is not sensitive to some variations of these parameters.

The proposed algorithm was successfully tested on various numerical samples. We will also show inversion from highly resolved diffraction measurements from Si lines on SiO₂/Si substrate and arrays of oxide-filled trenches in silicon (BM32 beamline, ESRF). The retrieved displacement fields with a resolution of about 8 nm are in excellent agreement with those calculated by finite element modelling based on continuum elasticity [4]. These results offer important perspective for local strain determination at the nanoscale. The work is currently concentrated on the investigation of the general applicability of the method to different types of structures in different geometries.

[1] J. R. Fienup, Appl. Opt. **21**, 2758 (1982); R. W. Gerchberg and W. O. Saxton, Optik (Stuttgart) **35**, 237 (1972).

[2] G. J. Williams, M. A. Pfeifer, I. A. Vartanyants, and I. K. Robinson, Phys. Rev. B **73**, 094112 (2006).

[3] A. A. Minkevich, M. Gailhanou, J.-S. Micha, B. Charlet, V. Chamard, and O. Thomas, submitted to Phys. Rev. Lett.

[4] M. Gailhanou, A. Loubens, J.-S. Micha, B. Charlet, A. A. Minkevich, R. Fortunier, and O. Thomas, accepted, to be published in Appl. Phys. Lett. **90** (2007).

^{*} Andrey.Minkevich@univ-cezanne.fr